Short Communication

Earth-Abundant SiX (X=S and Se) Monolayers as Promising Anode Materials for Lithium Ion Batteries, a First-Principles Study

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In this work, the adsorption energy, diffusion energy barrier and structural stability of Li on SiX (X=S and Se) monolayers were studied using density functional theory. The obtained adsorption energies were -3.41~2.54 eV and -3.13 ~ -2.39 eV for Li absorbed on the SiS and SiSe monolayers, respectively. SiX (X=S and Se) monolayers show larger adsorption energies than those of other two-dimensional materials such as graphene and the MoO₂ monolayer. The diffusion of Li depends on the diffusion direction, showing an anisotropic diffusion behaviour. Li prefers to diffuse along the valley with the energy barriers of 0.27 and 0.28 eV on the SiS and SiSe monolayers, respectively. The structure is maintained to form LiSiX (X=S and Se). The characteristics of large adsorption energy, small Li diffusion energy barrier, and high structural stability indicate that SiX (X=S and Se) monolayers can be used as a potential anode for lithium ion batteries.

Keywords: SiX (X=S and Se) monolayer, lithium ion batteries, adsorption energy, diffusion energy, structural stability, density functional theory

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